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14. ABSTRACT

While entanglement is believed to underlie the power of quantum computation and communication, it is not generally well understood for multipartite systems. Recently, it has been appreciated that there exists proper no-signaling probability distributions derivable from operators that do not represent valid quantum states. Such systems exhibit supra-correlations that are stronger than allowed by quantum mechanics, but less than the algebraically allowed maximum in Bell-inequalities (in the bipartite case). Some of these probability distributions are derivable from an entanglement witness W , which is a non-positive Hermitian operator constructed such that its expectation value with a separable quantum state (positive density matrix) ρ_{sep} is non-negative (so that $\text{Tr}[W \rho] < 0$ indicates entanglement in quantum state ρ). In the bipartite case, it is known that by a modification of the local no-signaling measurements by spacelike separated parties A and B, the supra-correlations exhibited by any W can be modeled as derivable from a physically realizable quantum state ρ . However, this result does not generalize to the n -partite case for $n > 2$. Supracorrelations can also be exhibited in 2- and 3-qubit systems by explicitly constructing "states" O (not necessarily positive quantum states) that exhibit PR correlations for a fixed, but arbitrary number, of measurements available to each party. In this paper we examine the structure of "states" that exhibit supra-correlations. In addition, we examine the affect upon the distribution of the correlations amongst the parties involved when constraints of positivity and purity are imposed. We investigate circumstances in which such "states" do and do not represent valid quantum states.

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Nonlocality, Entanglement Witnesses and Supra-correlations

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ABSTRACT

While entanglement is believed to underlie the power of quantum computation and communication, it is not generally well understood for multipartite systems. Recently, it has been appreciated that there exists proper no-signaling probability distributions derivable from operators that do not represent valid quantum states. Such systems exhibit *supra-correlations* that are stronger than allowed by quantum mechanics, but less than the algebraically allowed maximum in Bell-inequalities (in the bipartite case). Some of these probability distributions are derivable from an entanglement witness W , which is a non-positive Hermitian operator constructed such that its expectation value with a separable quantum state (positive density matrix) ρ_{sep} is non-negative (so that $\text{Tr}[W \rho] < 0$ indicates entanglement in quantum state ρ). In the bipartite case, it is known that by a modification of the local no-signaling measurements by spacelike separated parties A and B , the supra-correlations exhibited by any W can be modeled as derivable from a physically realizable quantum state ρ . However, this result does not generalize to the n -partite case for $n > 2$. Supra-correlations can also be exhibited in 2- and 3-qubit systems by explicitly constructing “states” O (not necessarily positive quantum states) that exhibit PR correlations for a fixed, but arbitrary number, of measurements available to each party. In this paper we examine the structure of “states” that exhibit supra-correlations. In addition, we examine the affect upon the distribution of the correlations amongst the parties involved when constraints of positivity and purity are imposed. We investigate circumstances in which such “states” do and do not represent valid quantum states.

Keywords: quantum entanglement, quantum non-locality, non-signaling theories, Popescu-Rohrlich boxes, EPR

1. INTRODUCTION

Physics imposes limits on the correlations that can be observed by distant (i.e. spacelike separated) parties. In particular, special relativity (SR) implies the principle of no-signaling (NS), that is correlations cannot lead to any sort of instantaneous communication between spacelike separated observers. Quantum correlations may be stronger than classical, and their violation of Bell inequalities¹ (BI) suggest that quantum mechanics (QM) cannot be regarded as a local realism theory. Tsirelson² showed that there is an upper bound to the violation of BI, which implies that the amount of non-locality allowed by QM is limited. Popescu and Rohrlich (PR) showed³ that there exists a broad class of no-signaling theories which allow stronger-than-quantum or *supra-quantum correlations*. PR developed a valid joint probability distribution whose violation of the BI lie above those of physical quantum correlations and below the allowed algebraic maximum of the BI (the latter are called PR-Boxes). Thus, the principle of NS imposed by SR does not single out QM from these other post-quantum NS theories⁴ (PQNS).

These PQNS have much in common with QM such as no-cloning, information-disturbance tradeoffs, security for key distribution, and others. Recently, van Dam⁵ showed that PR-Boxes make communication complexity trivial, which is not the case within QM. Other researchers have shown that PQNS theories would lead to implausible simplification of distributed computational tasks (see Pawłowski⁶ and references therein). It is now widely believed that theories in which communication/computational complexity is trivial are very unlikely to exist. It is therefore important to understand the structure of the PQNS and ultimately to find physical and informational principles that rule them out. In this paper we take steps in that direction by investigating the structure of PR correlations by forming operators which reproduce these PR probability distributions. We investigate circumstances in which they do and do not represent valid quantum states.

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2. BELL INEQUALITIES, PR BOXES AND SUPRA-QUANTUM CORRELATIONS

2.1 Bell Inequalities (BI)

Nonlocality is expressed by means of violations Bell inequalities¹ (BI) which set upper bounds for classical correlations arising from local-realistic theories. For bipartite systems, the most well know BI is the Clauser-Horne-Shimony-Holt (CHSH) inequality⁷ defined as follows. Consider a bipartite system $\mathcal{A} \otimes \mathcal{B}$, Alice and Bob, each possessing measurement directions $A, B \in \mathcal{A}$ and $C, D \in \mathcal{B}$ taking measurement values $a, b, c, d = \{\pm 1\}$. We define the correlation $E(AC)$ between $A \in \mathcal{A}$ and $C \in \mathcal{B}$ as

$$\begin{aligned} E(AC) &\equiv \langle AC \rangle = \sum_{a,c=\{\pm 1\}} a c P(a, c | A, C) \\ &= P(+, + | A, C) + P(-, - | A, C) - P(+, - | A, C) - P(-, + | A, C) \end{aligned} \quad (1)$$

In (1), we define $P(a, c | A, C)$ as the joint probability that given the (inputs) measurement directions A for Alice and C for Bob, Alice obtains the (outputs) measurement result a and Bob obtains the value b , subject to the normalization condition $\sum_{a,c=\{\pm 1\}} P(a, c | A, C) = 1, \forall A, C$. Finally, we define the following CHSH correlation parameter S by

$$S \equiv E(AC) + E(BC) + E(BD) - E(AD). \quad (2)$$

S has been cleverly constructed as the expectation value of the quantity $\text{Arg} \equiv A(C-D) + B(C+D)$. If A, B, C, D are classical random variables taking values ± 1 then it can be readily seen that if (i) $C=D$, then $|\text{Arg}| = |B(2C)| = 2$ and if (ii) $C=-D$, $|\text{Arg}| = |A(2D)| = 2$. Thus, for classical correlation we have the CHSH inequality

$$\text{CHSH inequality: } |S = E(AC) + E(BC) + E(BD) - E(AD)| \leq S_{\text{Cl}} = 2 \quad (3)$$

(where the subscript “Cl” denotes “classical”). For a large class of measurement directions (but not all), quantum states can violate the CHSH inequality (i.e. $|S| > 2$) up to a maximum value shown by Tsirelson² to be $S_Q = 2\sqrt{2}$. Here, a *quantum state* is defined as a positive (i.e. non-negative eigenvalues) Hermitian matrix with unit trace denoted by the symbol ρ . The archetypical example is the singlet (Bell) state

$$\rho_{\text{singlet}} = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) / \sqrt{2} \equiv (|01\rangle - |10\rangle) / \sqrt{2} \quad (4)$$

with measurement directions in the x - y plane: $A = \hat{x}, B = \hat{y}, C = (\hat{x} + \hat{y}) / \sqrt{2}, D = (\hat{x} - \hat{y}) / \sqrt{2}$ that saturates the Tsirelson bound with $S = -S_Q = -2\sqrt{2}$. This is a manifestation of the stronger than classical correlations that can be exhibited by quantum states. (Note: quantum states with measurement directions such that the CHSH inequality is satisfied, i.e. $S \leq 2$, are not distinguishable from classical states by the correlation parameter S).

It is instructive to note that the CHSH inequality in (3) can be derived⁸ as a statement of a classical quadrilateral inequality for the *correlation metric* $\Delta(AC) = 1 - E(AC) = P(+, - | A, C) + P(-, + | A, C) \geq 0$. Substituting this expression into (3) yields $\Delta(AC) + \Delta(BC) + \Delta(BD) \geq \Delta(AD) \Rightarrow S \equiv E(AC) + E(BC) + E(BD) - E(AD) \leq +2$ (see Fig. 1). Thus, the

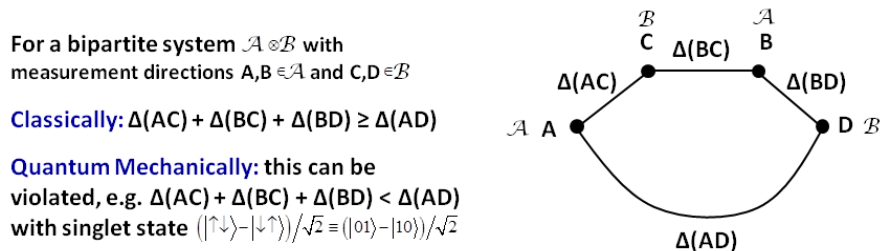


Fig.1 CHSH inequality derived as a violation of the classical quadrilateral inequality.

violation of the CHSH inequality by quantum states can be interpreted as a violation of the classical quadrilateral inequality which, for certain measurement directions, yields the distance $\Delta(AD)$ via the direct path $A-D$ to be *smaller* than the sum of the distances around the indirect path $A-C-B-D$.

Returning to the CHSH inequality (3), one notes that it is bounded by the algebraic maximum $|S| \leq S_{AM}=4$. This follows from the fact that the correlations E are bounded by $|E| \leq 1$. This latter result can be inferred by writing $E = P_{++} + P_{--} - (P_{+-} + P_{-+}) = 2(P_{++} + P_{--}) - 1 = 1 - 2(P_{+-} + P_{-+})$, where $P_{++} + P_{--} + P_{+-} + P_{-+} = 1$ has been used. Using the fact that $0 \leq P_{++} + P_{--} \leq 1$ and $0 \leq P_{+-} + P_{-+} \leq 1$ in the previous two expressions for E , yields the desired bound $|E| \leq 1$. Therefore, if the first three correlations in (3) take the value ± 1 and the last correlation takes the value ∓ 1 , we obtain $S = \pm 4$. The implication of this observation is that the regime $2\sqrt{2} \leq S \leq 4$ represents *supra-correlations* that are stronger than quantum, yet are unphysical by Tsirelson's bound, i.e. cannot be realized by any physical quantum state. The salient question to study is what 'natural' principles determine the exclusion of such supra-correlations. As a first hypothesis, one might surmise that the principle of *no-signaling* from special relativity (i.e. that information cannot be instantaneously broadcast between spacelike separated observers) might exclude supra-correlations. Surprisingly, this is *not* the case. In 1994, Popescu and Rohrlich³ (PR) were able to construct a valid joint probability distribution between a pair of spacelike separated observers that (i) satisfies the non-signaling principle, and (ii) yields the algebraic maximum correlations allowed by the CHSH inequality. Here the adjective 'valid' implies that the joint probability distribution, and all its derived marginal probability distributions obtain values between 0 and 1, and satisfy the appropriated normalization requirements (i.e. the joint and all marginal probability distributions summed over all outcomes for any measurement settings yields unity). These correlations are now called *PR correlations*, which we describe in the next section.

2.2 No Signaling (NS) Theories and PR Correlations

We wish to consider correlations between n spacelike separated parties (observers) A_1, \dots, A_n , who can perform m possible measurements x_1, \dots, x_n ($x_i = \{0, 1, \dots, m-1\}$), with r possible outcomes a_1, \dots, a_n ($a_i = \{0, 1, \dots, r-1\}$). The observed correlations will be described by the joint probability distribution $P(a_1, a_2, \dots, a_n | x_1, \dots, x_n)$ giving the probability that the parties obtain the measurement values (outputs) a_1, \dots, a_n when their local measurement apparatuses (inputs) are set to x_1, \dots, x_n . The joint probability distribution is constrained only by the conditions $0 \leq P(a_1, a_2, \dots, a_n | x_1, \dots, x_n) \leq 1$ and the normalization condition $\sum_{a_1, \dots, a_n} P(a_1, a_2, \dots, a_n | x_1, \dots, x_n) = 1$ for all measurement settings x_1, \dots, x_n .

Imposing the no-signaling (NS) constraint, i.e. adherence to the requirement from special relativity that spacelike separated measurements should not influence each other due to the finite speed of light (communication), requires that the marginal probability distributions satisfy the additional condition

$$\text{No Signaling: } P(a_1, a_2, \dots, a_k | x_1, \dots, x_n) \equiv \sum_{a_{k+1}, \dots, a_n \in \{0,1\}} P(a_1, \dots, a_n | x_1, \dots, x_n) = P(a_1, a_2, \dots, a_k | x_1, \dots, x_k). \quad (5)$$

Here, the first equality in (5) formally defines the marginal probability distribution describing the measurement outcomes of the first k parties, when the last $n-k$ outcomes are un-observed and hence summed over. Note, this marginal probability distribution $P(a_1, a_2, \dots, a_k | x_1, \dots, x_n)$ formally depends on all n measurement settings. The last equality in (5) imposes the NS constraint requiring that the marginal probability depends *only* upon the k measurement settings of the parties participating in the joint measurement (and not on the remaining $n-k$ measurement setting of the unobserved outcomes).

As first pointed out by Popescu and Rohrlich³, the NS constraint (5) by itself does not single out classical and quantum theories, i.e. $|S| \leq S_Q$. PR proposed the following joint probability distribution for two parties (Alice and Bob) with two measurement settings (inputs) $x, y = \{0, 1\}$, and two measurement outcomes (outputs) $a, b = \{0, 1\}$ given by

$$\text{PR Box: } P(a, b | x, y) = \begin{cases} 1/2 & \text{if } a \oplus b = x \cdot y \\ 0 & \text{otherwise} \end{cases}. \quad (6)$$

By considering all possible inputs and outputs, it is straightforward to show that PR correlations of (6) satisfy all the requirements for a NS theory as follows: normalization (total probability)

$$\begin{aligned}
& \sum_{a,b \in \{0,1\}} P(a,b | x, y) \\
&= \underbrace{P(0,0 | x, y) + P(1,1 | x, y)}_{a \oplus b = 0} + \underbrace{P(0,1 | x, y) + P(1,0 | x, y)}_{a \oplus b = 1}, \\
&= (1/2 + 1/2) \delta_{0,x \cdot y} + (1/2 + 1/2) \delta_{1,x \cdot y}, \\
&= \delta_{0,x \cdot y} + \delta_{1,x \cdot y}, \\
&= 1 \quad \forall x, y,
\end{aligned} \tag{7}$$

and the NS constraint

$$\begin{aligned}
P(a | x, y) &\equiv \sum_{b \in \{0,1\}} P(a,b | x, y) \\
&= \underbrace{P(a,0 | x, y)}_{a \oplus b = a \oplus 0 = a} + \underbrace{P(a,1 | x, y)}_{a \oplus b = a \oplus 1 = \bar{a}} \\
&= 1/2 \delta_{a, x \cdot y} + 1/2 \delta_{\bar{a}, x \cdot y}, \\
&= \begin{cases} 1/2 + 0 & (\text{if } a = 0 \& x \cdot y = 0), 0 + 1/2 & (\text{if } a = 0 \& x \cdot y = 1) \\ 0 + 1/2 & (\text{if } a = 1 \& x \cdot y = 0), 1/2 + 0 & (\text{if } a = 1 \& x \cdot y = 1) \end{cases}, \\
&= 1/2 \quad \forall a, x, y, \\
&= P(a | x) \quad \forall a, x \quad (\Rightarrow \text{Isotropic, i.e. } P(a | x) = 1/2 \text{ indep of } a, x).
\end{aligned} \tag{8}$$

With the PR Box define above in (6) we can compute correlations as

$$\begin{aligned}
E(a,b | x, y) &= \underbrace{P(0,0 | x, y) + P(1,1 | x, y)}_{a \oplus b = 0} - \underbrace{P(0,1 | x, y) + P(1,0 | x, y)}_{a \oplus b = 1}, \\
&= (1/2 + 1/2) \delta_{0,x \cdot y} - (1/2 + 1/2) \delta_{1,x \cdot y}, \\
&= \begin{cases} +1 & \text{if } x \cdot y = 0, \text{ i.e. } (x, y) \in \{(0,0), (0,1), (1,0)\}, \\ -1 & \text{if } x \cdot y = 1, \text{ i.e. } (x, y) = (1,1), \end{cases}
\end{aligned} \tag{9}$$

where we have used $E(a,b | x, y) = \sum_{a',b' \in \{\pm 1\}} a' b' P(a,b | x, y)$, where $a' = 1 - 2a$ ($b' = 1 - 2b$) associates the measurement values $a' (b') \in \{+1, -1\}$ with the measurement value labels (bits) $a (b) \in \{0,1\}$, respectively. Therefore, in Fig. 1, assigning Alice's measurement directions $A, B = \mathcal{A}$ the bit labels $x_A = 1$ and $x_B = 0$, and Bob's measurement directions $C, D = \mathcal{B}$ the bit labels $y_C = 0$ and $y_D = 1$, and using (9) yields the algebraic maximum $S_M = 4$ of the CHSH inequality, as illustrated in Fig. 2.

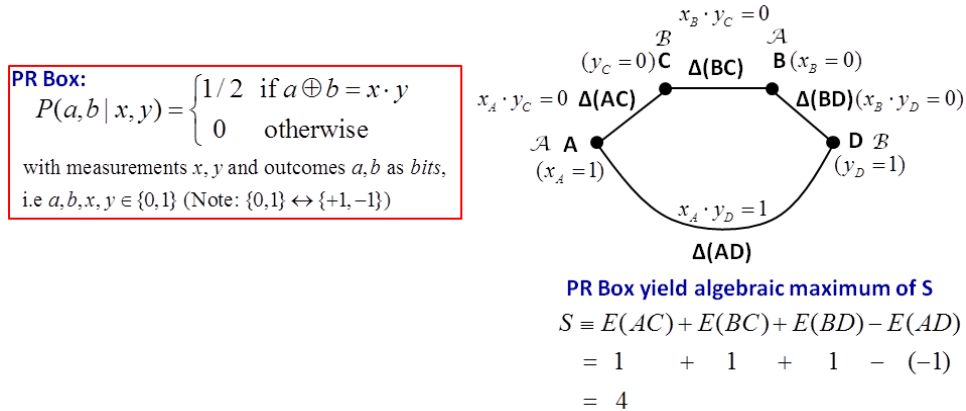


Fig.2 PR Box with joint probability distribution achieving the algebraic maximum $S_M = 4$ of the CHSH inequality.

Since $S_M=4>S_Q=2\sqrt{2}$, no quantum (i.e. physically realizable) state can reproduce the above PR probability (6). However, the following “state”⁹ $O = \alpha_+ |\Phi^+\rangle\langle\Phi^+| + \alpha_- |\Phi^-\rangle\langle\Phi^-|$ with $\alpha_{\pm} = (1 \pm \sqrt{2})/2$ and Bell states $|\Phi^{\pm}\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}$, yields the PR probability (6) through the usual trace rule $P_{PR}(a, b | x, y) = \text{Tr}[O M_a^x \otimes M_b^y]$ with $\{M_a^{x_A}, M_a^{x_B}\} = \{\sigma_2, \sigma_1\}$ and $\{M_b^{x_C}, M_b^{x_D}\} = \{(\sigma_1 + \sigma_2)/\sqrt{2}, (\sigma_1 - \sigma_2)/\sqrt{2}\}$, where $\{\sigma_i\}_{i \in \{1,2,3\}}$ are the usual Pauli matrices. Note that the form of the joint measurement between Alice and Bob written as a pure tensor product of local observables $M_a^x \otimes M_b^y$, ensures the locality of the spacelike separated measurements, which cannot increase entanglement between the parties. (A measurement involving the sum of pure tensor products, such as $M_a^x \otimes M_b^y + M_a'^x \otimes M_b'^y$ which might possibly create entanglement, would involve non-local measurements between the parties, which could only be physically realized if the parties were brought together). The important point is that O does not represent a physical quantum state since it is non-positive, i.e. it possesses the negative eigenvalue $\alpha_- = (1 - \sqrt{2})/2$. Henceforth, we shall refer to non-positive, unit trace Hermitian operators O capable of producing NS probability distributions as “states,” and reserve the specific term “quantum state” or “q-state” for the physically realizable positive, unit trace Hermitian operators denoted as $\rho \geq 0$, (i.e. density matrix).

Following Acin *et al.*⁹ we now wish to investigate all sets of n -party spacelike correlations in terms of local quantum observables (measurements) $M_{\text{non-sig}} = M_{a_1}^{x_1} \otimes \dots \otimes M_{a_n}^{x_n}$ that ensure NS. These correlations can be written in the form

$$P_O \equiv P_O(a_1, \dots, a_n | x_1, \dots, x_n) = \text{Tr}[O M_{a_1}^{x_1} \otimes \dots \otimes M_{a_n}^{x_n}]. \quad (10)$$

Without loss of generality, we can take the local measurement operators $M_a^x = \Pi_a^x = |a\rangle_x \langle a|$ to be the projection operators onto “spin-component” a in the “direction” x . Requiring that proper probabilities be derived from *all* local quantum measurements imposes the condition that O be positive on *all* product states. This implies that $O=W$ is an entanglement witness¹⁰ (EW) with the property $\langle \alpha, \beta, \dots | W | \alpha, \beta, \dots \rangle \geq 0$. Here some definition are helpful. A q-state is separable (contains only classical correlations) if it is of the form $\rho^{\text{sep}} = \sum_i p_i \rho_i^{A_1} \otimes \rho_i^{A_2} \otimes \dots \otimes \rho_i^{A_n}$ where each $\rho_i^{A_k}$ is a local density matrix and $\sum_i p_i = 1$. (If a q-state is not separable, it is entangled). Each local density matrix has a (non-unique) ensemble decomposition $\rho_i^{A_k} = \sum_j p_{ij}^k |\psi_{ij}^k\rangle\langle\psi_{ij}^k|$ where $\sum_j p_{ij}^k = 1$. The requirement that W is positive on all product states $\langle \alpha, \beta, \dots | W | \alpha, \beta, \dots \rangle \geq 0$ ensures that $\text{Tr}[\rho^{\text{sep}} W] \geq 0$ from the form of ρ^{sep} . A q-state ρ such that $\text{Tr}[\rho W] < 0$ is then entangled (since it is not separable), and W is said to “witness” (or exhibit) the entanglement of ρ . Note that W is in general a non-positive Hermitian operator. In the context of (10), we now consider $O \rightarrow W$ as a state (not necessarily a q-state) from which to derive NS correlations through the joint probability distributions

$$P_W \equiv P(a_1, \dots, a_n | x_1, \dots, x_n) = \text{Tr}[W M_{a_1}^{x_1} \otimes \dots \otimes M_{a_n}^{x_n}] \geq 0. \quad (11)$$

The correlations (11) are termed *Gleason correlations* by Acin *et al.*⁹

The subtle distinction between (10) and (11) is that the latter produces positive probabilities for *all* local NS measurements, while the former may produce non-negative probabilities on only a *subset* of NS measurements. This distinction is important since it has been shown^{10,11} that for bipartite systems $n=2$, any Gleason correlation $P(a_1, a_2 | x_1, x_2) = \text{Tr}[W M_{a_1}^{x_1} \otimes M_{a_2}^{x_2}] \geq 0$ can be converted to a probability distribution derived from a q-state $\rho_{|\Phi_{PB}\rangle} = |\Phi_{PB}\rangle\langle\Phi_{PB}|$ with modified measurements $P(a_1, a_2 | x_1, x_2) = \text{Tr}[W M_{a_1}^{x_1} \otimes M_{a_2}^{x_2}] = \text{Tr}[\rho_{|\Phi_{PB}\rangle} M_{a_1}^{x_1} \otimes \bar{M}_{a_2}^{x_2}] \geq 0$. Here $|\Phi_{PB}\rangle$ is any pure bipartite state (not necessarily maximally entangled). The proof relies on the explicit use of the Choi-Jamiołkowski isomorphism^{10,11,12} (CJI) which allows any bipartite ($n=2$) witness W to be written as

$W^{(n=2)} \equiv (I \otimes \Lambda)(\rho_{|\Phi_{PB}\rangle})$, where Λ is a positive trace preserving map. In the above, $\bar{M}_{a_2}^{x_2} = \Lambda^*(M_{a_2}^{x_2})$ where Λ^* is the adjoint of the map Λ , i.e. $\text{Tr}[A \Lambda(B)] = \text{Tr}[\Lambda^*(A) B]$. The proof then follows directly as

$$\begin{aligned} P_W(a, b | x, y) &= \text{Tr}[W M_a^x \otimes M_b^y] = \text{Tr}[(I \otimes \Lambda)(\rho_{|\Phi_{PB}\rangle}) M_a^x \otimes M_b^y] \\ &= \text{Tr}[M_a^x \otimes M_b^y (I \otimes \Lambda)(\rho_{|\Phi_{PB}\rangle})] = \text{Tr}[M_a^x \otimes \Lambda^*(M_b^y) \rho_{|\Phi_{PB}\rangle}] = \text{Tr}[\rho_{|\Phi_{PB}\rangle} M_a^x \otimes \bar{M}_b^y], \end{aligned} \quad (12)$$

where the second equality uses the CJI, the third equality uses the cyclic property of the trace, the fourth inequality utilizes $I \otimes \Lambda$ acting to the left on the tensor product measurements $M_a^x \otimes M_b^y$ thereby introducing the adjoint Λ^* operation and the modified local measurement operation $\bar{M}_{a_2}^{x_2} = \Lambda^*(M_{a_2}^{x_2})$ in the last equality. Acin *et al.*⁹ point out that the CJI decomposition $W^{(N=2)} \equiv (I \otimes \Lambda)(\rho_{|\Phi_{PB}\rangle})$ in general fails for $n > 2$ (which they demonstrate by a specific example). Thus, the Gleason correlations (11) are strictly larger ($|S| > S_Q$) than quantum correlations for $n > 2$ (and equivalent only for $n \leq 2$). The state $O = \alpha_+ |\Phi^+\rangle\langle\Phi^+| + \alpha_- |\Phi^-\rangle\langle\Phi^-|$ used in the example of PR correlations in the discussion after Fig. 2 is *not* an EW since it can produce negative probabilities for measurements other than those considered (it would be an EW if it produced positive probabilities for *all* measurement choices). Acin *et al.*⁹ classify the distributions $P(a_1, \dots, a_n | x_1, \dots, x_n)$ as (i) *No-Signaling* if and only if P can be written in the form of (10), (ii) *Quantum* whenever O is positive ($O \geq 0$), and (iii) *Local* if and only if O corresponds to a separable quantum state. In the following, we investigate the NS correlations of (10) and the conditions for which they become either Gleason, or Quantum correlations.

2.3 No Signaling (NS) Correlations: 2-Qubits

Following Acin *et al.*⁹ we define an n -partite probability distribution $P(a_1, \dots, a_n | x_1, \dots, x_n)$ as being NS if and only if there exists local quantum measurements $M_{a_i}^{x_i}$ and a Hermitian operator O of unit trace such that (10) holds. It is important to note that O need not produce positive probabilities for other measurements outside this set. Acin *et al.*⁹ give a prescription for the formal construction of O given the set of measurements $M_{a_i}^{x_i}$. In the following we present an explicit construction for O for the case of $n=2$ qubits ($r=2$ outputs, i.e. $a, b = \{0, 1\}$) and arbitrary number m of measurement inputs ($x, y = \{0, 1, \dots, m-1\}$). Later, we extend this to the case of $n=3$ for qubits.

As stated in the previous section, without loss of generality we can take the local Hermitian measurement operators to be the projection operators onto “spin-component” a in the “direction” x , $M_a^x = \Pi_a^x = |a\rangle_x \langle a|$. For each x , the completeness of the measurement operators give $\sum_{a=0}^{r-1} M_a^x \equiv I_{r \times r}$ where $I_{r \times r} \equiv I$ is the $r \times r$ identity matrix. This allows us to write the $a=r-I$ measurement operator as $M_{a=r-1}^x \equiv I_{r \times r} - \sum_{a=0}^{r-2} M_a^x$. One defines the (tilde) Hermitian matrices \tilde{M}_a^x dual to M_a^x through the inner product $\text{Tr}[M_a^x \tilde{M}_{a'}^{x'}] = \delta_{x,x'} \delta_{a,a'}$. For the bipartite case $n=2$, with in general m measurement settings with r measurement outcomes, one has

$$O = \sum_{a,b=0}^{r-2} \sum_{x,y=0}^{m-1} P(a, b | x, y) \tilde{M}_a^x \otimes \tilde{M}_b^y + \sum_{a=0}^{r-2} \sum_{x=0}^{m-1} P(a | x) \tilde{M}_a^x \otimes \tilde{I} + \sum_{b=0}^{r-2} \sum_{y=0}^{m-1} P(b | y) \tilde{I} \otimes \tilde{M}_b^y + \tilde{I} \otimes \tilde{I}, \quad (13)$$

where \tilde{I} is the tilde matrix dual to the $r \times r$ identity matrix I , with the additional orthogonality conditions defined by $\text{Tr}[I \tilde{I}] = \text{Tr}[\tilde{I}] = 1$, $\text{Tr}[M_a^x \tilde{I}] = 0$, and $\text{Tr}[I \tilde{M}_{a'}^{x'}] = \text{Tr}[\tilde{M}_{a'}^{x'}] = 0$. The conditions ensure that O is Hermitian, $\text{Tr}[O]=1$ and probabilities are given by the trace formulas $P(a, b | x, y) = \text{Tr}[O M_a^x \otimes M_b^y]$, $P(a | x) = \text{Tr}[O M_a^x \otimes I]$ and $P(b | y) = \text{Tr}[O I \otimes M_b^y]$. This is illustrated in Fig. 3 where Alice and Bob share PR correlations by means of, what are termed in the literature, a pair of *PR boxes* (or NS {non-signaling} boxes).

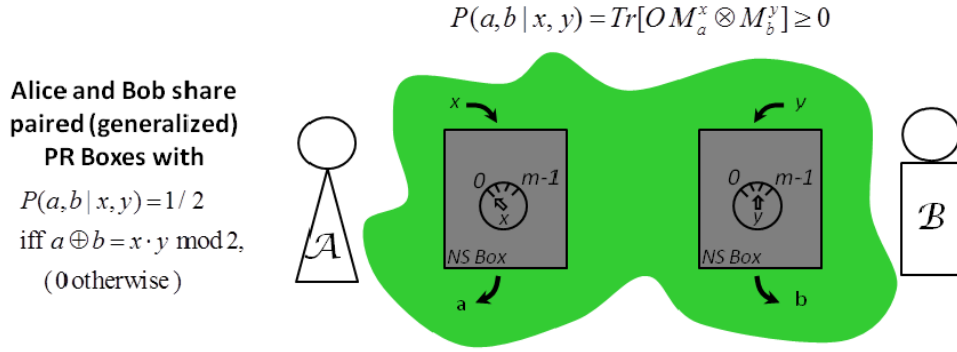


Fig.3 PR Box shared between Alice and Bob.

In the following we specialize to the case of qubits ($r=2$, $a, b = \{0, 1\}$) with arbitrary number m of measurement inputs ($x, y = \{0, 1, \dots, m-1\}$). In this case the measurement operators $M_{a=0}^x$ are given as projection operators for “spin-up” along the directions $x \rightarrow \vec{m}_x$ on the Bloch sphere. The $M_{a=0}^x$ are just density matrices on the Bloch sphere written as

$$M_{a=0}^x = |0\rangle_x \langle 0| = 1/2(I + \vec{m}_x \cdot \vec{\sigma}), \quad \vec{m}_x = m_x(\sin \theta_x \cos \phi_x, \sin \theta_x \sin \phi_x, \cos \theta_x) \quad (14)$$

$$|\vec{m}_x| \leq 1, \text{ (density matrix on Bloch Sphere),}$$

where $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of single qubit Pauli matrices. Although not required for the case of qubits, the projection onto “spin-down” along x is given by $M_{a=1}^x = |1\rangle_x \langle 1| = 1/2(I - \vec{m}_x \cdot \vec{\sigma}) = I - M_{a=0}^x$, with I the 2×2 identity matrix. Equation (13) now simplifies to the form

$$O = \sum_{x,y=0}^{m-1} P(a=0, b=0 | x, y) \tilde{M}_0^x \otimes \tilde{M}_0^y + \sum_{x=0}^{m-1} P(a=0 | x) \tilde{M}_0^x \otimes \tilde{I} + \sum_{y=0}^{m-1} P(b=0 | y) \tilde{I} \otimes \tilde{M}_0^y + \tilde{I} \otimes \tilde{I}. \quad (15)$$

We simplify the notation by defining $\{I, M_{a=0}^x; x=0, \dots, m-1\} \equiv \{M_{-1} \equiv I, \{M_{i \geq 0}\} = \{M_{-1}, M_0, M_1, \dots\}\} = \{M_{\alpha=\{-1, i \geq 0\}}\}$ (a set of $m+1$ linear independent matrices) with duals $\{\tilde{M}_{\beta=\{-1, j \geq 0\}}\} \equiv \{\tilde{M}_{-1} \equiv \tilde{I}, \tilde{M}_0, \tilde{M}_1, \dots\}$ satisfying the trace orthogonality conditions $\text{Tr}[M_\alpha \tilde{M}_\beta] = \delta_{\alpha, \beta}$, and similarly for $\{I, \{M_{j \geq 0}^y\}\} \rightarrow \{N_{\beta=\{-1, j \geq 0\}}\}$. We therefore write (15) as

$$O = \sum_{i,j=0}^{m-1} P_{i,j}^{0,0} \tilde{M}_i \otimes \tilde{N}_j + \sum_{i=0}^{m-1} P_i^{0,\bullet} \tilde{M}_i \otimes \tilde{I} + \sum_{j=0}^{m-1} P_j^{\bullet,0} \tilde{I} \otimes \tilde{N}_j + \tilde{I} \otimes \tilde{I}, \quad (16)$$

using the abbreviations $P_{i,j}^{0,0} = P(a=0, b=0 | x=i, y=j)$, $P_i^{0,\bullet} = P(a=0 | x=i)$ and $P_j^{\bullet,0} = P(b=0 | y=j)$. For the measurement matrices $M_{-1} = I \equiv I_{2 \times 2}$, and $M_{i \geq 0} = 1/2(I + \vec{m}_i \cdot \vec{\sigma})$, $|\vec{m}_i| \leq 1$, the dual matrices are given explicitly by $\tilde{M}_{-1} \equiv \tilde{I} = 1/2(I - \sum_{i \geq 0} \vec{m}_i \cdot \vec{\sigma}) \equiv 1/2(I - \vec{m} \cdot \vec{\sigma})$, and $\tilde{M}_i = \vec{m}_i \cdot \vec{\sigma}$ where $\vec{m}_i \cdot \vec{m}_j = \delta_{i,j}$, $|\vec{m}_i| \geq 1$, with the orthogonality relations $\text{Tr}[\tilde{I}] = 1$, $\text{Tr}[\tilde{M}_j] = 0$, $\text{Tr}[M_i \tilde{I}] = 0$, and $\text{Tr}[M_i \tilde{M}_j] = \delta_{i,j}$. Using the relationship $\text{Tr}[X \otimes Y] = \text{Tr}[X] \text{Tr}[Y]$ it is straightforward to verify that $\text{Tr}[O] = 1$ and, for example, $P_{i,j}^{0,0} = \text{Tr}[O M_i \otimes N_j]$ which picks out the term $\tilde{M}_i \otimes \tilde{N}_j$ in (16). Other probabilities are obtained for example as $P_{i,j}^{0,1} = \text{Tr}[O M_i \otimes (I - N_j)] = \text{Tr}[O M_i \otimes I] - \text{Tr}[O M_i \otimes N_j] = P_i^{0,\bullet} - P_{i,j}^{0,0} = \sum_{b=\{0,1\}} P_{i,j}^{0,b} - P_{i,j}^{0,0} = P_{i,j}^{0,1} = P(a=0, b=1 | x=i, y=j)$. Substituting the explicit expressions for the dual matrices into (16) yields the general expression for O in terms of products of Pauli matrices

$$O = \frac{1}{4} \left[\sum_{i,j=0}^{m-1} (4P_{i,j}^{0,0} - 2(P_i^{0,\bullet} + P_j^{\bullet,0}) + 1) (\vec{m}_i \cdot \vec{\sigma}) \otimes (\vec{n}_j \cdot \vec{\sigma}) + \sum_{i=0}^{m-1} (2P_i^{0,\bullet} - 1) (\vec{m}_i \cdot \vec{\sigma}) \otimes I + \sum_{j=0}^{m-1} (2P_j^{\bullet,0} - 1) I \otimes (\vec{n}_j \cdot \vec{\sigma}) + I \otimes I \right]. \quad (17)$$

Specializing to the PR correlations in (6) given by $P(a,b | x=i, y=j) = 1/2 \delta_{a \oplus b, i \cdot j \bmod 2} \Rightarrow P_{i,j}^{0,0} = 1/2 \delta_{0, i \cdot j \bmod 2}$ with marginals $P_i^{0,\bullet} = P_j^{\bullet,0} = 1/2 \forall i, j$, yields the expression for the NS PR operator

$$O_{PR} = \frac{1}{4} \left[(\vec{m}_e \cdot \vec{\sigma}) \otimes (\vec{n}_e \cdot \vec{\sigma}) + (\vec{m}_e \cdot \vec{\sigma}) \otimes (\vec{n}_o \cdot \vec{\sigma}) + (\vec{m}_o \cdot \vec{\sigma}) \otimes (\vec{n}_e \cdot \vec{\sigma}) - (\vec{m}_o \cdot \vec{\sigma}) \otimes (\vec{n}_o \cdot \vec{\sigma}) + I \otimes I \right], \quad (18)$$

where $\vec{m}_e = \sum_{i=0,1,2,\dots} \vec{m}_{2i}$, $\vec{m}_o = \sum_{i=0,1,2,\dots} \vec{m}_{2i+1}$, $\vec{n}_e = \sum_{j=0,1,2,\dots} \vec{n}_{2j}$, $\vec{n}_o = \sum_{j=0,1,2,\dots} \vec{n}_{2j+1}$.

In (18) the subscripts $\{e,o\}$ denote {even,odd} for the summation over even and odd dual measurement vectors. Note that in (18) the “single- σ ” terms $\sigma_i \otimes I$ and $I \otimes \sigma_j$ (representing measurements by Alice or Bob alone, respectively) have dropped out since the marginal distributions $P(a/x)=P(b/y)=1/2$ are independent of a,b,x,y . This leaves only the solely two-party correlation terms $\sigma_i \otimes \sigma_j$ and the maximally mixed term $(I \otimes I)/4$. For the bipartite case $n=2$ often considered in the literature for two qubits, each with two measurement directions $x \in \{\vec{m}_0, \vec{m}_1\}$ for Alice and $y \in \{\vec{n}_0, \vec{n}_1\}$ for Bob (i.e. $a,b,x,y \in \{0,1\}$) we obtain the simplified form

$$O'_{PR} = \frac{1}{4} \left[(\vec{m}_0 \cdot \vec{\sigma}) \otimes (\vec{n}_0 \cdot \vec{\sigma}) + (\vec{m}_0 \cdot \vec{\sigma}) \otimes (\vec{n}_1 \cdot \vec{\sigma}) + (\vec{m}_1 \cdot \vec{\sigma}) \otimes (\vec{n}_0 \cdot \vec{\sigma}) - (\vec{m}_1 \cdot \vec{\sigma}) \otimes (\vec{n}_1 \cdot \vec{\sigma}) + I \otimes I \right]. \quad (19)$$

Using the procedure for calculating probabilities discussed after equation (16), the following probabilities can be computed from (19)

$\vec{n}_0 \quad \vec{n}_1$	$\vec{n}_0 \quad \vec{n}_1$	$\vec{n}_0 \quad \vec{n}_1$	$\vec{n}_0 \quad \vec{n}_1$	$\vec{n}_0 \quad \vec{n}_1$
$\vec{m}_0 \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 0 \end{bmatrix}$	$\vec{m}_0 \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 0 \end{bmatrix}$	$\vec{m}_0 \begin{bmatrix} 0 & 0 \\ 0 & 1/2 \end{bmatrix}$	$\vec{m}_0 \begin{bmatrix} 0 & 0 \\ 0 & 1/2 \end{bmatrix}$	$\vec{m}_0 \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
$\vec{m}_1 \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 0 \end{bmatrix}$	$\vec{m}_1 \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 0 \end{bmatrix}$	$\vec{m}_1 \begin{bmatrix} 0 & 0 \\ 0 & 1/2 \end{bmatrix}$	$\vec{m}_1 \begin{bmatrix} 0 & 0 \\ 0 & 1/2 \end{bmatrix}$	$\vec{m}_1 \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$

$$P(a=0, b=0 | x=\vec{m}_i, y=\vec{n}_j), \quad P(a=1, b=1 | \vec{m}_i, \vec{n}_j), \quad P(a=0, b=1 | \vec{m}_i, \vec{n}_j), \quad P(a=1, b=0 | \vec{m}_i, \vec{n}_j), \quad E(\vec{m}_i, \vec{n}_j) \quad (20)$$

$a \oplus b = 0, \quad \quad \quad a \oplus b = 1,$

$\Rightarrow P = 1/2 \text{ for } (x, y) \in \{(0,0), (0,1), (1,0)\}, \quad \quad \quad \Rightarrow P = 1/2 \text{ for } (x, y) \in \{(1,1)\}.$

Here, the correlations in (20) are computed as (see (1))

$$E(\vec{m}_i, \vec{n}_j)_{i,j \in \{0,1\}} = P(a=0, b=0 | x=\vec{m}_i, y=\vec{n}_j) + P(a=1, b=1 | \vec{m}_i, \vec{n}_j) - P(a=0, b=1 | \vec{m}_i, \vec{n}_j) - P(a=1, b=0 | \vec{m}_i, \vec{n}_j), \quad (21)$$

with corresponding S parameter (see (2))

$$S = E(\vec{m}_0, \vec{n}_0) + E(\vec{m}_0, \vec{n}_1) + E(\vec{m}_1, \vec{n}_0) - E(\vec{m}_1, \vec{n}_1) = 4 = S_{AM}, \quad (22)$$

achieving the algebraic maximum value $S_{AM} = 4$.

For the case of two qubits with $m=3$ measurement vectors $x \in \{\vec{m}_0, \vec{m}_1, \vec{m}_2\}$ for Alice and $y \in \{\vec{n}_0, \vec{n}_1, \vec{n}_2\}$ for Bob (i.e. $a,b \in \{0,1\}$, with $x,y \in \{0,1,2\}$) we obtain from (18) the probabilities and correlations

$$\begin{array}{ccccc}
\vec{n}_0 & \vec{n}_1 & \vec{n}_2 & \vec{n}_0 & \vec{n}_1 & \vec{n}_2 & \vec{n}_0 & \vec{n}_1 & \vec{n}_2 & \vec{n}_0 & \vec{n}_1 & \vec{n}_2 & \vec{n}_0 & \vec{n}_1 & \vec{n}_2 \\
\vec{m}_0 \begin{bmatrix} 1/2 & 1/2 & 1/2 \end{bmatrix}, & \vec{m}_0 \begin{bmatrix} 1/2 & 1/2 & 1/2 \end{bmatrix}, & \vec{m}_0 \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}, & \vec{m}_0 \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}, & \vec{m}_0 \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} \\
\vec{m}_1 \begin{bmatrix} 1/2 & 0 & 1/2 \end{bmatrix}, & \vec{m}_1 \begin{bmatrix} 1/2 & 0 & 1/2 \end{bmatrix}, & \vec{m}_1 \begin{bmatrix} 0 & 1/2 & 0 \end{bmatrix}, & \vec{m}_1 \begin{bmatrix} 0 & 1/2 & 0 \end{bmatrix}, & \vec{m}_1 \begin{bmatrix} 1 & -1 & 1 \end{bmatrix} \\
\vec{m}_2 \begin{bmatrix} 1/2 & 1/2 & 1/2 \end{bmatrix}, & \vec{m}_2 \begin{bmatrix} 1/2 & 1/2 & 1/2 \end{bmatrix}, & \vec{m}_2 \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}, & \vec{m}_2 \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}, & \vec{m}_2 \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}
\end{array} \quad (23)$$

$$\begin{array}{ccccc}
P(a=0, b=0 | x=\vec{m}_i, y=\vec{n}_j), & P(a=1, b=1 | \vec{m}_i, \vec{n}_j), & P(a=0, b=0 | \vec{m}_i, \vec{n}_j), & P(a=1, b=0 | \vec{m}_i, \vec{n}_j), & E(\vec{m}_i, \vec{n}_j) \\
a \oplus b = 0, & a \oplus b = 1, & & & \\
\Rightarrow P = 1/2 \text{ for } (x, y) \in \{(e, e), (e, o), (o, e)\}, & \Rightarrow P = 1/2 \text{ for } (x, y) \in \{(o, o)\}.
\end{array}$$

In (23) $e = \{0, 2\}$ denotes even indices of the measurement directions while $o = \{1\}$ denotes odd indices. We achieve the algebraic maximum for the S parameter, generalizing (22) defined as

$$S = E(\vec{m}_e, \vec{n}_e) + E(\vec{m}_e, \vec{n}_o) + E(\vec{m}_o, \vec{n}_e) - E(\vec{m}_o, \vec{n}_o) = 4 = S_{AM}. \quad (24)$$

Note that the dimension of the measurement vectors \vec{m}_i is set by the dimension $D = d^2 - 1$ of the Hilbert space of the observer, which simply states that any $(D+1) \times (D+1)$ matrix can be written in term of the $(D+1) \times (D+1)$ identity matrix and the D generators of $su(d)$. For qubits, $D=3$ and the three generators of $su(2)$ are the usual Pauli matrices $\vec{\sigma}$. For a given set of m measurement 3-vectors $\{\vec{m}_i\}$ (vectors in the Bloch sphere, $|\vec{m}_i| \leq 1$) one needs to solve for the correspond dual measurement vectors $\{\vec{m}_j\}$ satisfying $\vec{m}_i \cdot \vec{m}_j = \delta_{i,j}$. We write these equations as the matrix equation

$\mathbf{M}_{m \times 3} \tilde{\mathbf{M}}_{3 \times m} = \mathbf{I}_{m \times m}$ where the i th row ($i = \{0, 1, \dots, m-1\}$) of (the known coefficient matrix) $\mathbf{M}_{m \times 3}$ is \vec{m}_i , and the j th column of (unknowns) $\tilde{\mathbf{M}}_{3 \times m}$ is \vec{m}_j . By linear algebra, there exists a right inverse of $\mathbf{M}_{m \times 3}$ via $\tilde{\mathbf{M}}_{\text{Right Inv}} = \mathbf{M}^T (\mathbf{M} \mathbf{M}^T)^{-1}$ (if $(\mathbf{M} \mathbf{M}^T)^{-1}$ exists) if the columns of $\mathbf{M}_{m \times 3}$ span R^m , which can only occur for $m \leq D=3$. The systems of equations is under-determined and there exists at least one solution (typically and infinite number due to undetermined free parameters). This is the situation for probabilities and correlations shown in (20) and (23) for the case $m=2$ and $m=3$ measurement vectors, respectively. For the $m > D=3$, there exists at most one, unique solution (if any). This is the least squares (LS) solution using the pseudo-inverse $\mathbf{M}_{m \times 3}$ given by $\tilde{\mathbf{M}}_{LS} = (\mathbf{M}^T \mathbf{M})^{-1} \mathbf{M}^T$ (if $(\mathbf{M}^T \mathbf{M})^{-1}$ exists). In general, the LS solution has non-zero residual errors given by $\mathbf{Err} = \mathbf{M}_{m \times 3} \tilde{\mathbf{M}}_{LS(3 \times m)} - \mathbf{I}_{m \times m}$, corresponding to joint probabilities that may be negative for some measurements but still satisfy the (total probability) normalization condition $\sum_{a,b} P(a, b | x, y) = 1, \forall x, y$. Nonetheless, it is instructive to perform numerical searches in the case of $m > 3$ of random measurement vectors to seek solutions which yield all joint probabilities in the range $0 \leq P(a, b | x, y) \leq 1$, for all pairs of measurement vectors \vec{m}_i, \vec{n}_j for Alice and Bob that still yield supra-correlations, i.e. $0 < S - S_Q \leq 4 - 2\sqrt{2} = 1.172$.

For the case $m=4$, a particular solution is shown in (25) that yields $S - S_Q = 0.102$ (for brevity, we only show $P(a=0, b=0 | x=\vec{m}_i, y=\vec{n}_j)$ and the correlations $E(\vec{m}_i, \vec{n}_j)$). In general, the even/odd structure of the correlations $E(\vec{m}_i, \vec{n}_j)$

$$\begin{array}{cccc}
\vec{n}_0 & \vec{n}_1 & \vec{n}_2 & \vec{n}_3 \\
\vec{m}_0 \begin{bmatrix} 0.237 & 0.395 & 0.072 & 0.406 \end{bmatrix}, & \vec{m}_0 \begin{bmatrix} -0.052 & 0.581 & -0.710 & 0.623 \end{bmatrix} \\
\vec{m}_1 \begin{bmatrix} 0.162 & 0.018 & 0.381 & 0.004 \end{bmatrix}, & \vec{m}_1 \begin{bmatrix} -0.350 & -0.927 & 0.522 & -0.982 \end{bmatrix} \\
\vec{m}_2 \begin{bmatrix} 0.469 & 0.449 & 0.341 & 0.457 \end{bmatrix}, & \vec{m}_2 \begin{bmatrix} 0.875 & 0.796 & 0.365 & 0.829 \end{bmatrix} \\
\vec{m}_3 \begin{bmatrix} 0.249 & 0.038 & 0.481 & 0.024 \end{bmatrix}, & \vec{m}_3 \begin{bmatrix} -0.004 & -0.847 & 0.923 & -0.905 \end{bmatrix}
\end{array} \quad (25)$$

$$\begin{array}{cc}
P(a=0, b=0 | x=\vec{m}_i, y=\vec{n}_j), & E(\vec{m}_i, \vec{n}_j)
\end{array}$$

exhibited in the cases $m \leq 3$ ((20) and (23)) is destroyed, yet they still produce supra-correlations $S - S_Q \geq 0$. For each value of m in Fig. 4 (left) we searched 10^5 random trials of the measurement vectors $\{\vec{m}_i, \vec{n}_j\}_{i,j \in \{0,1,\dots,m-1\}}$ and plot the value of $S -$

S_Q for the first solution encountered in which (i) we find proper joint probability distributions $0 \leq P(a, b | x = \vec{m}_i, y = \vec{n}_j) \leq 1$ for all measurement vectors, and (ii) which produce supra-correlations, $S - S_Q \geq 0$. In Fig. 4 (middle), we plot the minimum

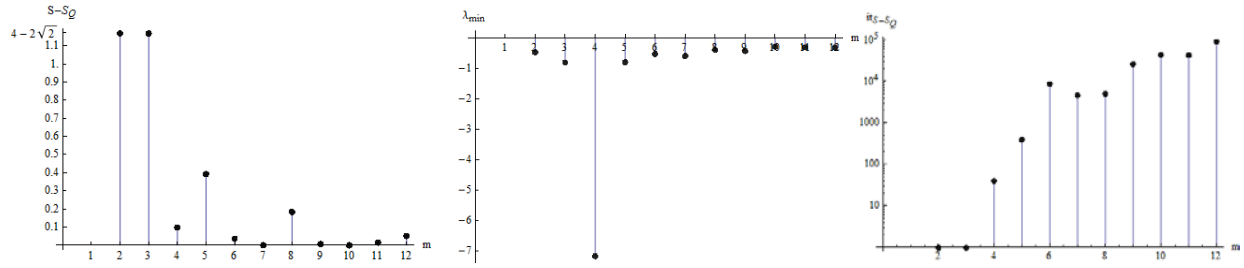


Figure 4. (left) Numerical simulations for $m=\{2,3,4,\dots,12\}$ measurement vectors yielding valid joint probabilities $0 \leq P(a, b | x = \vec{m}_i, y = \vec{n}_j) \leq 1$ for all pairs of measurement vectors $\{\vec{m}_i, \vec{n}_j\}_{i,j \in \{0,1,\dots,m-1\}}$ and supra-correlations $S - S_Q > 0$. (middle) Minimum eigenvalue λ_{\min} of O in (18). The negative values indicates that O is not a proper quantum state (positive, Hermitian operator, $\rho \geq 0$). (right) Iteration number (out of 10^5 random trials) at which the first set of m measurements vectors were found for Alice and Bob producing supra-correlation shown in the leftmost figure.

eigenvalue λ_{\min} of the matrix O in (18). The negative value of λ_{\min} indicates that O is not realized by a proper quantum state (i.e. a positive, Hermitian operator, $\rho \geq 0$). The rightmost plot in Fig. 4 is the iteration number at which the first set of measurement vectors was found which produced supra-correlations. For the values of $13 \leq m \leq 20$ numerically explored, no supra-correlations solutions were found within 10^5 trials (the plot indicates that it becomes exponentially hard to find such a solution).

2.4 No Signaling (NS) Correlations: 3-Qubits

The bipartite results of the previous section for $n=2$ -qubits are straightforwardly extended to the tripartite case of $n=3$ -qubits with similar implications. Here the generalization of the bipartite CHSH nonlocality parameter S is given by the Svetlichny¹³ inequality (SI) relating correlations $E(a, b, c | x, y, z)$ between three spacelike separated parties A, B, C

$$S \equiv E(a, b, c | 0, 0, 0) + E(a, b, c | 0, 1, 0) + E(a, b, c | 1, 0, 0) - E(a, b, c | 1, 1, 0) \\ + E(a, b, c | 0, 0, 1) - E(a, b, c | 0, 1, 1) - E(a, b, c | 1, 0, 1) - E(a, b, c | 1, 1, 1). \quad (26)$$

The SI has the bounds (i) $|S| \leq S_C = 4$ for classical correlations, (ii) $|S| \leq S_Q = 4\sqrt{2}$ for quantum correlations, with (iii) the algebraic upper bound given by $|S| \leq S_{AM} = 8$, achieved when the correlations in (26) take the values $E=1$ if they are preceded by a plus sign, and $E=-1$ if they are preceded by a minus sign. The generalization of the PR correlations of (6) is given by¹⁴

$$\text{TPR Box: } P(a, b, c | x, y, z) = \begin{cases} 1/4 & \text{if } a \oplus b \oplus c = x \cdot y \oplus y \cdot z \oplus x \cdot z, \\ 0 & \text{otherwise} \end{cases}, \quad (27)$$

often referred to as a tripartite PR (TPR) box. The marginal distributions of (27) are again isotropic and satisfy the NS constraint, i.e. $P(a, b, c | x, y, z) = P(a, b | x, y) = 1/4$ for all a, b, x, y, z and $P(a, c | x, y) = P(a | x) = 1/2$ for all a, x, y , and similarly for all other marginal probability distributions.

For the case of $n=3$ qubits ($r=2$ output measurement values) $a, b, c = \{0, 1\}$, with m possible measurement vectors for each observer, $x, y, z = \{0, 1, \dots, m-1\}$ we again find that only the highest (three party) correlations term and the maximally mixed term are non-zero in the expression for O_{TPR}

$$O_{TPR} = \frac{1}{8} \left[\{(\vec{m}_e \cdot \vec{\sigma}) \otimes (\vec{n}_e \cdot \vec{\sigma}) + (\vec{m}_e \cdot \vec{\sigma}) \otimes (\vec{n}_o \cdot \vec{\sigma}) + (\vec{m}_o \cdot \vec{\sigma}) \otimes (\vec{n}_e \cdot \vec{\sigma}) - (\vec{m}_o \cdot \vec{\sigma}) \otimes (\vec{n}_o \cdot \vec{\sigma})\} \otimes (\vec{r}_e \cdot \vec{\sigma}) \right. \\ \left. - \{(\vec{m}_o \cdot \vec{\sigma}) \otimes (\vec{n}_o \cdot \vec{\sigma}) + (\vec{m}_o \cdot \vec{\sigma}) \otimes (\vec{n}_e \cdot \vec{\sigma}) + (\vec{m}_e \cdot \vec{\sigma}) \otimes (\vec{n}_o \cdot \vec{\sigma}) - (\vec{m}_e \cdot \vec{\sigma}) \otimes (\vec{n}_e \cdot \vec{\sigma})\} \otimes (\vec{r}_o \cdot \vec{\sigma}) + I \otimes I \otimes I \right], \quad (28)$$

where $\vec{q}_e = \sum_{i=0,1,2,\dots} \vec{q}_{2i}$, $\vec{q}_o = \sum_{i=0,1,2,\dots} \vec{q}_{2i+1}$, $\vec{q} = \{\vec{m}, \vec{n}, \vec{r}\}$.

The regular, even/odd (mod 2) structure of O_{TPR} in (28) reflects the non-zero structure of the TRP probabilities in (27), and can be seen as an additional single qubit generalization of O_{PR} in (18). That is, the 2-qubit term in the first curly brackets in (28) $\{(\vec{m}_e \cdot \vec{\sigma}) \otimes (\vec{n}_e \cdot \vec{\sigma}) + (\vec{m}_e \cdot \vec{\sigma}) \otimes (\vec{n}_o \cdot \vec{\sigma}) + (\vec{m}_o \cdot \vec{\sigma}) \otimes (\vec{n}_e \cdot \vec{\sigma}) - (\vec{m}_o \cdot \vec{\sigma}) \otimes (\vec{n}_o \cdot \vec{\sigma})\}$ tensor-producted with the remaining “even” qubit term $(\vec{r}_e \cdot \vec{\sigma})$, is precisely two-party correlation term that appears in O_{PR} in (18). Similarly, the term in the second curly bracket in (28) $\{(\vec{m}_o \cdot \vec{\sigma}) \otimes (\vec{n}_o \cdot \vec{\sigma}) + (\vec{m}_o \cdot \vec{\sigma}) \otimes (\vec{n}_e \cdot \vec{\sigma}) + (\vec{m}_e \cdot \vec{\sigma}) \otimes (\vec{n}_o \cdot \vec{\sigma}) - (\vec{m}_e \cdot \vec{\sigma}) \otimes (\vec{n}_e \cdot \vec{\sigma})\}$ tensor-producted with the remaining “odd” qubit term $(\vec{r}_o \cdot \vec{\sigma})$ (with the accompanying minus sign) is just the bit flip ($e \leftrightarrow o$) of the previous two-party correlation term. Again, we can achieve the algebraic maximum $S_{AM}=8$ when each party has (for the case of qubits) at most $m=3$ measurement vectors (for exactly the same linear algebraic reason for the $n=2$ bipartite case). Further, as in the bipartite case, we can find particular NS supra-correlation solutions $0 < S - S_Q \leq 4 - 2\sqrt{2}$ for $m > 3$, but which become increasingly hard to find the larger the value of m .

3. POSITIVITY AND PURITY CONSTRAINTS ON QUANTUM CORRELATIONS

In general, any n -qubit $2^n \times 2^n$ matrix can be decomposed into the sum of tensor products of at most n Pauli matrices with the 2×2 identity matrix I . For the bipartite case composed of $n=2$ qubits we can write the matrix $O^{(n=2)}$ as^{15,16}

$$O^{(2)} = \frac{1}{4} \left[I \otimes I + (\vec{s}^{(1)} \cdot \vec{\sigma}) \otimes I + I \otimes (\vec{s}^{(2)} \cdot \vec{\sigma}) + \sum_{\alpha, \beta=1}^3 C_{\alpha\beta} \sigma_\alpha \otimes \sigma_\beta \right]. \quad (29)$$

Here $\vec{s}^{(1)}$ and $\vec{s}^{(2)}$ are the vectors on the Bloch sphere representing Alice’s and Bob’s single-party properties respectively, and the 3×3 matrix $C_{\alpha\beta} = \text{Tr}[O \sigma_\alpha \otimes \sigma_\beta]$ encode the 2-party, joint correlations between Alice and Bob. Here we have used

$$\sigma_\mu \sigma_\nu = \delta_{\mu\nu} I + i \varepsilon_{\mu\nu\lambda} \sigma_\lambda, \quad \text{and} \quad \text{Tr}[I/2] = 1. \quad (30)$$

From (17) and (18) $\vec{s}^{(1)} = \vec{s}^{(2)} = 0$ with the PR correlation matrix given by $C_{\alpha\beta}^{PR} = \sum_{i,j=0}^{m-1} (4P_{i,j}^{0,0} - 1) (\vec{m}_i)_\alpha \otimes (\vec{n}_j)_\beta$, where $P_{i,j}^{0,0} = 1/2 \delta_{0,i \cdot j \bmod 2}$, and hence $(4P_{i,j}^{0,0} - 1) = 1$ if $i \cdot j \bmod 2 = 0$, and -1 otherwise. The essential feature of PR correlation matrix is reflected in the coefficient $(4P_{i,j}^{0,0} - 1)$ involving the PR probabilities, which reproduces the rightmost 3×3 matrix $E(\vec{m}_i, \vec{n}_j)$ in (23) for the case $m=3$ (which is the well-posed case with 3 equations for 3 unknowns given the \vec{m}_i , for the dual measurement vectors \vec{m}_j satisfying $\vec{m}_i \cdot \vec{m}_j = \delta_{i,j}$, possessing a unique solution). Thus, it is reasonable to drop the requirement that the set of fixed measurement vectors $\{\vec{m}_i\}$ and $\{\vec{n}_j\}$ are predetermined, and agreed upon by Alice and Bob, and consider instead the solely two-party correlated state

$$O_{PR} = \frac{1}{4} \left[I \otimes I + \sum_{\alpha, \beta=1}^3 C_{\alpha\beta}^{PR} \sigma_\alpha \otimes \sigma_\beta \right], \quad C_{\alpha\beta}^{PR} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, \quad \Rightarrow E(\vec{m}, \vec{n}) = \sum_{\alpha, \beta=1}^3 m_\alpha C_{\alpha\beta}^{PR} \otimes n_\beta \equiv \vec{m} \cdot \mathbf{C}^{PR} \cdot \vec{n}. \quad (31)$$

Equation (31) yields supra-correlations that achieve the algebraic maximum $S_{AM}=4$ with the choice e.g. $\{\vec{m}_{i=\{0,1,2\}}\} = \{\hat{x}, \hat{y}, \hat{z}\} = \{\vec{n}_{j=\{0,1,2\}}\}$ (amongst many possibilities). However, for arbitrary measurement vectors $\{\vec{m}_i\}$ and $\{\vec{n}_j\}$ the

correlations are bounded by $|E(\vec{m}, \vec{n})| \leq 2\sqrt{2}$ (in numerical simulations, by 2.551 in 10^5 random trials), which can lead to negative probabilities since e.g. $P(a=0, b=0 | x=\vec{m}, y=\vec{n}) = 1/4(1 + E(\vec{m}, \vec{n}))$. If one scales $C_{\alpha\beta}^{PR} \rightarrow C_{\alpha\beta}^{PR} / (2\sqrt{2})$ so that $|E(\vec{m}, \vec{n})| \leq 1$, the probabilities are now bounded between 0 and $1/2$, and O_{PR} becomes an entanglement witness (a non-positive Hermitian operator that is positive on all product states), but an uninteresting one, since the value of the nonlocality parameter is reduced from $S_{AM}=4$ to $S_{AM}/2\sqrt{2} = \sqrt{2} < S_{CL}=2$.

As relevant comparison to O_{PR} , the density matrix for the quantum singlet Bell state $|\psi^{\text{singlet}}\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$ is given by

$$\rho^{\text{singlet}} = \frac{1}{4} \left[I \otimes I + \sum_{\alpha, \beta=1}^3 C_{\alpha\beta}^{\text{singlet}} \sigma_{\alpha} \otimes \sigma_{\beta} \right], \quad C_{\alpha\beta}^{\text{singlet}} = -\delta_{\alpha\beta} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \Rightarrow E^{\text{singlet}}(\vec{m}, \vec{n}) = -\vec{m} \cdot \vec{n}, \quad (32)$$

(note, the other three maximally entangled Bell states also have diagonal 2-party correlation matrices with two +1, and one -1 matrix elements). ρ^{singlet} is a valid quantum (pure) state with eigenvalues $\{1, 0, 0, 0\}$, while O_{PR} is not, since it possess a negative eigenvalue $(1 - \sqrt{17})/4$. The question at hand is what governs the structure of the 2-party correlation matrix $C_{\alpha\beta}$? In the following, we consider the constraints of both positivity (i.e. non-negative eigenvalues) and purity (i.e. is quantum state pure) on O_{PR} .

For completeness, we note that the tripartite PR box O_{TPR} in (28) is of the solely three-party correlation form

$$O_{TPR} = \frac{1}{8} \left[I \otimes I \otimes I + \sum_{\alpha, \beta, \gamma=1}^3 C_{\alpha\beta\gamma}^{TPR} \sigma_{\alpha} \otimes \sigma_{\beta} \otimes \sigma_{\gamma} \right], \quad (33)$$

which is a special case of the $n=3$ qubit state $O^{(n=3)}$

$$O^{(3)} = \frac{1}{8} [I \otimes I \otimes I + (\vec{s}^{(1)} \cdot \vec{\sigma}) \otimes I \otimes I + I \otimes (\vec{s}^{(2)} \cdot \vec{\sigma}) \otimes I + I \otimes I \otimes (\vec{s}^{(3)} \cdot \vec{\sigma}) + \sum_{\alpha, \beta=1}^3 A_{\alpha\beta} \sigma_{\alpha} \otimes \sigma_{\beta} \otimes I + \sum_{\alpha, \beta=1}^3 B_{\alpha\beta} \sigma_{\alpha} \otimes I \otimes \sigma_{\beta} + \sum_{\alpha, \beta=1}^3 C_{\alpha\beta} I \otimes \sigma_{\alpha} \otimes \sigma_{\beta} + \sum_{\alpha, \beta, \gamma=1}^3 C_{\alpha\beta\gamma} \sigma_{\alpha} \otimes \sigma_{\beta} \otimes \sigma_{\gamma}]. \quad (34)$$

Again, the pertinent question is what governs the distribution of the correlations amongst single parties ($\vec{s}^{(i)}$), two parties $A_{\alpha\beta}, B_{\alpha\beta}, C_{\alpha\beta}$, and three-parties $C_{\alpha\beta\gamma}$.

3.1 Positivity constraints

In an extensive review of 2-qubit states of the form (29), Englert and Metwally¹⁶ derive constraints amongst the single and two-party correlations imposed by the (positivity) condition that $O^{(2)} \geq 0$. Here we generalize their arguments to an arbitrary n -qubit state $O^{(n)}$ defined by

$$O^{(n)} = \frac{1}{N} [I \otimes I \otimes \dots \otimes I + (\vec{s}^{(1)} \cdot \vec{\sigma}) \otimes I \otimes \dots \otimes I + \dots + I \otimes \dots \otimes I \otimes (\vec{s}^{(n)} \cdot \vec{\sigma}) + \sum_{\alpha_1, \alpha_2=1}^3 C_{\alpha_1\alpha_2}^{(1,2)} \sigma_{\alpha_1} \otimes \sigma_{\alpha_2} \otimes I \otimes \dots \otimes I + \dots + \sum_{\alpha_{n-1}, \alpha_n=1}^3 C_{\alpha_{n-1}\alpha_n}^{(n-1,n)} I \otimes \dots \otimes I \otimes \sigma_{\alpha_{n-1}} \otimes \sigma_{\alpha_n} + \dots + \sum_{\alpha_1, \alpha_2, \dots, \alpha_n=1}^3 C_{\alpha_1\alpha_2\dots\alpha_n}^{(1,2,\dots,n)} \sigma_{\alpha_1} \otimes \sigma_{\alpha_2} \otimes \dots \otimes \sigma_{\alpha_n}] \equiv \frac{1}{N} [I_N - K], \quad (35)$$

where $I_N = I \otimes I \otimes \dots \otimes I$ is the $N \times N$ identity matrix with $N = 2^n$, and K is the traceless part of $O^{(n)}$ (noting $\text{Tr}[\sigma_i] = 0$) given by

$$K = I - N O^{(n)} \quad (N = 2^n), \quad O^{(n)} \geq 0 \Rightarrow K \leq I. \quad (36)$$

K contains all the terms in $O^{(n)}$ except the maximally mixed term I_N/N . If $O^{(n)} \geq 0$ (all eigenvalues are non-negative) then the eigenvalues of K are all less than unity by (36). Now, the eigenvalues $\{\lambda_{i=1,\dots,N}\}$ of any $N \times N$ complex matrix A are determined by its characteristic equation $\chi_A(\lambda) = \prod_{i=1}^N (\lambda - \lambda_i) = 0$. By the Cayley-Hamilton theorem¹⁷, A satisfies its own (matrix) characteristic equation, i.e. $\chi_A(A) = 0$. This can be used to develop a set of recursion relations¹⁸ relating the coefficients of the characteristic (N th degree) polynomial $\chi_A(\lambda)$ to traces of the powers of A denoted by $T_m \equiv \text{Tr}[A^m]$

$$\chi_A(\lambda) = \lambda^N + D_1 \lambda^{N-1} + \dots + D_{N-1} \lambda + D_N \Rightarrow mD_m + D_{m-1}T_1 + D_{m-2}T_2 + \dots + D_1T_{m-1} + T_m = 0, \quad m = 1, 2, \dots, N. \quad (37)$$

The last term in (37) allows one to recursively solve for D_m as $mD_m = -\sum_{k=1}^m T_k D_{m-k}$ (defining $D_0 \equiv 0$). Specializing to the traceless case $A=K$ of (36), we have $T_1 = \text{Tr}[K] = 0$. For the $n=2$ -qubit case ($N=4$) we have

$$n = 2, N = 2^n = 4: \quad D_2 = -1/2 T_2, \quad D_3 = -1/3 T_3, \quad D_4 = -1/4 [T_4 - 1/2 T_2^2]. \quad (38)$$

Note that expressions D_m for an arbitrary number of qubits n do not require a recalculation of previously computed expression of the D_m for fewer number $n' < n$ of qubits.

We now note the following useful observation: since $\chi_A(K) = 0$, and by (36) each eigenvalue is less than unity $\{\lambda_{i=1,\dots,N} \leq 1\}$, it follows that $\chi_A(\lambda) = \prod_{i=1}^N (\lambda - \lambda_i) \geq 0$ and is monotonically increasing for $\lambda \geq 1$. This further implies the same is true for all derivatives of the characteristic polynomial i.e. $(d\chi_A^k(\lambda)/d\lambda^k)_{\lambda \geq 1} \geq 0$, for $k = 0, 1, \dots, N$. Thus, taking derivatives of the characteristic polynomial written in the form $\chi_A(\lambda) = \sum_{k=0}^N D_{N-k} \lambda^k$ and evaluating at $\lambda = 1$ allows us to define $N-1$ non-trivial positivity conditions (for derivatives $k = 2, \dots, N$) in the compact form

$$\sum_{r=2}^k \binom{N-r}{N-k} (-D_r) \leq \binom{N}{k} = \frac{N!}{k!(N-k)!}, \quad (39)$$

to determine when $O^{(n)} \geq 0$ for the case of n -qubits. Using (39) with the relations in (38) for $k=2,3,4$ yields

$$T_2 \leq N(N-1); \quad (N-2)(T_2/2) + (T_3/3) \leq \binom{N}{3}; \quad \frac{(N-2)(N-3)}{2}(T_2/2) + (N-3)(T_3/3) + 1/4(T_4 - 1/2 T_2^2) \leq \binom{N}{4}. \quad (40)$$

The D_2 constraint on $T_2 = \text{Tr}[K^2]$ (first inequality in (40)), can be further simplified. For the general n -qubit state $O^{(n)}$ the non-zero contributions to T_2 come from the square of each individual term, yielding a common factor of $N = \text{Tr}[I_N]$

$$\begin{aligned} T_2 = \text{Tr}[K^2] &= N \left[\sum_{i=1}^n (\bar{s}^{(i)})^2 + \sum_{i < j} \sum_{\alpha_1, \alpha_2=1}^3 (C_{\alpha_1 \alpha_2}^{(i,j)})^2 + \dots + \sum_{\alpha_1, \alpha_2, \dots, \alpha_n=1}^3 (C_{\alpha_1 \alpha_2 \dots \alpha_n}^{(1,2,\dots,n)})^2 \right] \leq N(N-1) \\ \Rightarrow n=2: \quad \bar{s}^{2(1)} + \bar{s}^{2(2)} + \sum_{\alpha_1, \alpha_2=1}^3 C_{\alpha_1 \alpha_2}^2 &\leq (N-1)_{N=2^2} = 3, \\ \Rightarrow n=3: \quad \bar{s}^{2(1)} + \bar{s}^{2(2)} + \bar{s}^{2(3)} + \sum_{\alpha_1, \alpha_2=1}^3 A_{\alpha_1 \alpha_2}^2 + \sum_{\alpha_1, \alpha_2=1}^3 B_{\alpha_1 \alpha_2}^2 + \sum_{\alpha_1, \alpha_2=1}^3 C_{\alpha_1 \alpha_2}^2 + \sum_{\alpha_1, \alpha_2, \alpha_3=1}^3 C_{\alpha_1 \alpha_2 \alpha_3}^2 &\leq (N-1)_{N=2^3} = 7, \end{aligned} \quad (41)$$

where we have illustrated the specific cases of $n=2$ from (29), and $n=3$ from (34). Equation (41) can be intuitively understood as follows. The first line of (41) indicates that there are $N-1 = 2^n - 1$ ways to distribute correlations in the state $O^{(n)}$: $\binom{n}{1} = n$ single-party correlations $\vec{s}^{(1)}, \vec{s}^{(2)}, \dots, \vec{s}^{(n)}$, $\binom{n}{2} = n(n-1)/2$ two-party correlations $C_{\alpha_1 \alpha_2}^{(i,j)}$ for $1 \leq i \leq j \leq n$ etc..., up to $\binom{n}{n} = 1$ n -body correlations. The sum of all these correlation repositories is $\sum_{k=1}^n \binom{n}{k} = 2^n - 1 = N - 1$.

We can now make some quantitative observations. From (31), the $n=2$ qubits PR state $O^{(2)}$ has $\vec{s}^{(1)} = \vec{s}^{(2)} = 0$, with all the correlations in the two-party correlation term $C_{\alpha\beta}^{PR}$ containing 9 non-zero entries. Thus, $\sum_{\alpha\beta=1}^3 (C_{\alpha\beta}^{PR})^2 = 9$ violates the $n=2$ T_2 positivity constraint $\sum_{\alpha\beta=1}^3 (C_{\alpha\beta})^2 \leq 3$ in (41). The supra-correlation PR joint probability distribution in (6) gives rise to more correlations in $C_{\alpha\beta}^{PR}$ that are allowed physically by nature. On the other hand, note that the quantum singlet state in (32) with $C_{\alpha\beta}^{\text{singlet}} = -\delta_{\alpha\beta}$ not only satisfies, by also saturates the T_2 positivity constraint (as do the other three maximally entangled Bell states).

As a counter example, for $n=3$ the state $O_{TPR;\varepsilon}$ from (33), defined by setting $C_{\alpha\beta\gamma}^{TPR;\varepsilon} \equiv \varepsilon_{\alpha\beta\gamma}$ (the Levi-Civita anti-symmetric symbol with value +1 for even permutations of (1,2,3), and -1 for odd permutations) has 6 non-zero entries, and therefore does satisfies the $n=3$ T_2 constraint $\sum_{\alpha,\beta,\gamma=1}^3 (C_{\alpha\beta\gamma}^{TPR;\varepsilon})^2 = 6 < 7$ in (41). However, $O_{TPR;\varepsilon}$ is a non-positive operator, and thus not a quantum state. To discriminate the non-positivity of this state, we must turn to the D_3 positivity constraint (the second inequality in (40); $k=3$ in (39)). In computing $T_3 = \text{Tr}[K^3]$ for $O_{TPR;\varepsilon}$ one must form the product of three Pauli matrices for each qubit $\sigma_\alpha \sigma_\beta \sigma_\gamma = i \varepsilon_{\alpha\beta\gamma} I + \delta_{\alpha\beta} \sigma_\gamma - \delta_{\alpha\gamma} \sigma_\beta + \delta_{\beta\gamma} \sigma_\alpha$ with $\text{Tr}[\sigma_\alpha \sigma_\beta \sigma_\gamma] = 2i \varepsilon_{\alpha\beta\gamma}$, which is purely imaginary. For the odd number $n=3$ qubits in $O_{TPR;\varepsilon}$, the product of three such traces in the calculation of T_3 is proportional to $i^3 = -i$. Since K is Hermitian with real eigenvalues, the same is true for all positive powers K^m , so that T_m in general must be real. Thus, symmetry relations in the triple summations involved in computing T_3 conspire to yield $T_3 = 0$. The same is true for the trace of any odd power of K in $O_{TPR;\varepsilon}$, i.e. $T_{2m+1} = \text{Tr}[K^{2m+1}] = 0$, since (i) for each qubit, traces of odd number of Pauli σ -matrices are proportional to i and (ii) for an odd number $2n'+1$ of qubits, the product of an odd number of such individual qubit traces is proportional to $i^{2n'+1}$ which is again imaginary. In fact, $T_{2m+1} = 0$ is true for any odd number qubit state $O^{(2n'+1)}$ that involves solely $(2n'+1)$ -party correlations (i.e. only the first and last terms in (35)). Substituting $T_3 = 0$ into (40) leads to the more restrictive constraint $T_2 \leq N(N-1)/3$ which translates into $\sum_{\alpha,\beta,\gamma=1}^3 (C_{\alpha\beta\gamma})^2 \leq 7/3$, which is violated by $\sum_{\alpha,\beta,\gamma=1}^3 (C_{\alpha\beta\gamma}^{TPR;\varepsilon})^2 = 6$ for $O_{TPR;\varepsilon}$. Since the tripartite PR state is of the form O_{TPR} in (33) one might try to achieve the algebraic maximum of the Svetlichny inequality by requiring all 8 terms in (26) to be of equal magnitude c . The above constraint would require $\sum_{\alpha,\beta,\gamma=1}^3 (C_{\alpha\beta\gamma})^2 = 8c^2 \leq 7/3$ or $c = 1/2\sqrt{7/6}$ if the bound is saturated. But then the Svetlichny inequality would be bounded by $S_{Cl} < |S| = 8c = 4\sqrt{7/6} < S_Q$. Thus the correlations could be quantum, i.e. stronger than classical, but not supra-correlations (stronger than quantum).

3.2 Purity constraints

The n -qubit state $O^{(n)}$ (35) is called *pure* if it is a rank one projector, i.e. $O_{\text{pure}}^{(n)} = |\Psi_N\rangle\langle\Psi_N|$ for normalized N -vector $|\Psi_N\rangle$, or equivalently, the condition $O_{\text{pure}}^{2(n)} = O_{\text{pure}}^{(n)}$ holds, i.e. $O_{\text{pure}}^{(n)}(O_{\text{pure}}^{(n)} - I_N) = 0$. Upon writing $O^{(n)} = 1/N[I_N - K]$ the purity condition becomes

$$\text{Pure State: } O_{\text{pure}}^{(n)} (O_{\text{pure}}^{(n)} - I_N) = 0 \Rightarrow K^2 = (N-1)I_N - (N-2)K. \quad (42)$$

Taking the trace in (42) yields $T_2 = N(N-1)$ which saturates the upper bound of the first (D_2) positivity inequality in (40). Multiplying (42) by K^m and taking the trace yields the recursion relation $T_{m+2} = (N-1)T_m - (N-2)T_{m+1}$ which can be used to express T_m as functions of N : $T_3 = -N(N-1)(N-2)$, $T_4 = N(N-1)^2 + N(N-1)(N-2)^2$, etc... These in turn can be used to explicitly show that the pure states saturate the upper bound of the positivity constraints (40), and consequently all the positivity constraints (39). As an immediate consequence, states such as O_{TPR} in (33) and their generalization, involving an odd number $n = 2n' + 1$ of qubits and solely n -party correlations, cannot be pure due to the fact that all odd traces $T_{2n'+1} = 0$ from the discussion in the previous section. This is not necessarily the case for states involving solely n -party correlations when n is even. Important particular instances are the $n=2$ -qubit maximally entangled Bell states involving solely 2-party correlations, of the which the singlet state in (32) is a representative example.

The purity constraint (42) forces relationships amongst the correlations, determining how they are distributed amongst the parties. An explicit construction of (42) for the general 2-qubit state $O^{(2)}$ (29) yields the relations $s_\alpha^{(1)} = \sum_{\beta=1}^3 C_{\alpha\beta} s_\beta^{(2)}$, $s_\beta^{(2)} = \sum_{\alpha=1}^3 s_\alpha^{(1)} C_{\alpha\beta}$, and $C_{\alpha\beta} = s_\alpha^{(1)} s_\beta^{(2)} - C_{\alpha\beta}^{(sub)}$ where $C_{\alpha\beta}^{(sub)} \equiv 1/2 \sum_{\mu\nu\mu'\nu'=1}^3 C_{\mu\nu} C_{\mu'\nu'} \epsilon_{\mu\mu'\alpha} \epsilon_{\nu\nu'\beta}$ (the matrix of cofactors of $C_{\alpha\beta}$). For the Bell states $s_\alpha^{(1)} = s_\beta^{(2)} = 0$, so that the purity condition requires the 2-party correlations to obey $C_{\alpha\beta} = -C_{\alpha\beta}^{(sub)}$. Englert and Metwally¹⁶ have shown that the generic $n=2$ -qubit quantum state $O^{(2)} = \rho^{(2)} \geq 0$ (29) is of the form

$$n = 2 \text{ qubit pure quantum state: } \rho_{\text{pure}}^{(2)} = 1/4 [I \otimes I + p \sigma_1 \otimes I + p I \otimes \sigma_1 - \sigma_1 \otimes \sigma_1 - q \sigma_2 \otimes \sigma_2 - \sigma_3 \otimes \sigma_3] \geq 0, \quad (43)$$

where $0 \leq p \leq 1$ is the common length of the individual Bloch vectors $\vec{s}^{(1)}$ and $\vec{s}^{(2)}$, and $q = \sqrt{1-p^2} \geq 0$ is the concurrence¹⁹ (a complete measure of two qubit entanglement for both pure and mixed quantum states). For the case of pure quantum states (43) the concurrence is given by $q^2 = \text{Tr}[\rho_{\text{pure}}^{(2)*} \rho_{\text{pure}}^{(2)}]$, where $\rho_{\text{pure}}^{(2)*}$ is the complex conjugate of $\rho_{\text{pure}}^{(2)}$.

For $n=3$ qubit pure states $O^{(3)}$ with general form (34), the distribution of the correlations amongst the various parties is much more complex. From the discussion above we know the correlations in (34) cannot be solely 3-party correlations, implying that some of the correlations must also be distributed amongst 1-party and/or 2-party combinations. Recently, much research has concentrated on the study of the relation between nonlocality, embodied in the Svetlichny parameter S in (26)), and pure state entanglement as measured by Wootters tangle²⁰ τ . The tangle between qubits 1, 2 and 3 is defined by

$$0 \leq \tau = \mathcal{C}_{1(23)}^2 - \mathcal{C}_{12}^2 - \mathcal{C}_{13}^2 \leq 1. \quad (44)$$

In (44) the concurrence¹⁹ \mathcal{C}_{12} quantifies the bipartite entanglement between qubit 1 and 2 after qubit 3 has been traced out, and similarly for \mathcal{C}_{13} . The concurrence $\mathcal{C}_{1(23)}$ measures the bipartite entanglement between the two subsystems composed of (i) qubit 1 and (ii) qubits 2 and 3 taken together. The reduced density matrix $\rho_{23} = \text{Tr}_1[\rho_{123}]$ can be shown to have two non-zero eigenvalues and hence acts as an effective single qubit whose bipartite entanglement with qubit 1 is measured by $\mathcal{C}_{1(23)} = 2\sqrt{\text{Tr}[\rho_1]}$ (for the case of a pure 3-qubit quantum state). The concurrence \mathcal{C} between two qubits described by the quantum state ρ is given by¹⁹ $\mathcal{C} = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$ where λ_i are the square roots of the eigenvalues, in decreasing order, of the matrix $\tilde{\rho}\tilde{\rho}$ where $\tilde{\rho} = (\sigma_2 \otimes \sigma_2) \rho^* (\sigma_2 \otimes \sigma_2)$.

Ghose *et al.*²¹ have investigated the relationship between the maximum value S_{max} of the Svetlichny parameter for a given value of the tangle τ for a class of three parameter 3-qubit states defined by $|\phi\rangle = \cos \theta_1 |000\rangle + \sin \theta_1 |\phi_1 \phi_2 \phi_3\rangle$ with

$|\phi_1\rangle = |1\rangle$, $|\phi_2\rangle = \cos\theta_2|0\rangle + \sin\theta_2|1\rangle$, and $|\phi_3\rangle = \cos\theta_3|0\rangle + \sin\theta_3|1\rangle$. The state $|\phi\rangle$ has tangle $\tau = (\sin 2\theta_1 \sin \theta_2 \sin \theta_3)^2$. Some important special cases of these three parameter states are (i) the maximally sliced (MS) states, of which there are two types, $|MS_2\rangle$ and $|MS_3\rangle$ and (ii) the generalized GHZ state $|GGHZ\rangle$ given by

$$\begin{aligned} |MS_2\rangle &= \frac{1}{\sqrt{2}}(|000\rangle + \cos\theta_2|101\rangle + \sin\theta_2|111\rangle), \quad |MS_3\rangle = \frac{1}{\sqrt{2}}(|000\rangle + \cos\theta_3|110\rangle + \sin\theta_3|111\rangle); \\ |GGHZ\rangle &= \cos\theta_1|000\rangle + \sin\theta_1|111\rangle, \text{ with } \tau_{MS_2}^2 = \sin^2\theta_2, \tau_{MS_3}^2 = \sin^2\theta_3, \tau_{GGHZ}^2 = \sin^2 2\theta_1. \end{aligned} \quad (45)$$

Emery and Beenaker²² have established bounds on S_{\max} for a given three tangle as $|\frac{1}{16}S_{\max}^2 - 1| \leq \tau \leq \frac{1}{32}S_{\max}^2$ for the MS states. Ghose *et al.*²¹ have established the bound as $S_{\max}^{(MS)} = 4\sqrt{1+\tau^{(MS)}}$. For the GHZ state Ghose *et al.*²¹ have established the bounds $S_{\max}^{(GGHZ)} = 4\sqrt{1-\tau^{(GGHZ)}}$ for $\tau \leq 1/3$ and $S_{\max}^{(GGHZ)} = 4\sqrt{2\tau^{(GGHZ)}}$ for $\tau \geq 1/3$. All three states in (45) achieve the maximum tangle $\tau=1$ on the GHZ state $|GHZ\rangle = 1/\sqrt{2}(|000\rangle + |111\rangle)$ (the generalization of the symmetric Bell state $|\Phi^+\rangle = 1/\sqrt{2}(|00\rangle + |11\rangle)$) which also achieves the maximum nonlocality $S=S_Q=4\sqrt{2}$ for a quantum state.

To examine how the correlations are distributed amongst the parties for the states in (45) let us denote $s_i^2 = \bar{s}^{2(i)}$ for the square of the 1-party correlations in (34), $C_{12}^2 = \sum_{\alpha\beta=1}^3 A_{\alpha\beta}^2 = \text{Tr}[A^T A]$, $C_{13}^2 = \text{Tr}[B^T B]$, $C_{23}^2 = \text{Tr}[C^T C]$ as the sum of the squares of the 2-party correlations, and $C_{123}^2 = \sum_{\alpha\beta\gamma=1}^3 C_{\alpha\beta\gamma}^2$ as the sum of the squares of the 3-party correlations. The state $|MS_3\rangle$ has correlations distributed such that (i) $s_1^2 = s_2^2 = 0$, $s_3^2 = 1 - \tau$, (ii) $C_{12}^2 = 3 - 2\tau$, $C_{13}^2 = C_{23}^2 = \tau$, and (iii) $C_{123}^2 = 3 + \tau$, with $\tau = \sin^2\theta_3$. Maximum tangle $\tau = 1$ on the GHZ state arranges the correlations so that (i) all the 1-party correlations are zero, (ii) $C_{12}^2 = C_{13}^2 = C_{23}^2 = 1$ and (iii) $C_{123}^2 = 4$ is maximized. This is the same behavior as the state $|\psi_{\text{Svetlichny}}\rangle = 1/2(-|000\rangle + |011\rangle + |101\rangle + |110\rangle)$ that Svetlichny¹³ put forth as an example of a state that achieves maximum nonlocality $S=S_Q$. This is in contrast to another important class of 3-qubits states, the W state²³, with $\tau = 0$, defined by $W = 1/\sqrt{3}(|100\rangle + |010\rangle + |001\rangle)$ in which (i) the only non-zero 1-party correlations are $s_3^{(1)} = s_3^{(2)} = s_3^{(3)} = 1/3$, (ii) all 2-party correlation matrices are identical $C_{12} = C_{13} = C_{23} = \text{diagonal}[2/3, 2/3, -1/3]$ and (iii) the non-zero 3-party correlations are given by $(C_{123})_{\alpha\beta\gamma} = 2/3$ for $\alpha\beta\gamma = \{113, 131, 223, 232, 312, 321\}$ and $(C_{123})_{333} = -1$. For the generalized GHZ state $|GGHZ\rangle$ (i) $s_3^{(1)} = s_3^{(2)} = s_3^{(3)} = \sqrt{1-\tau}$ with $\tau = \sin^2 2\theta_1$ so that $s_1^2 + s_2^2 + s_3^2 = 3 - 3\tau$, (ii) $C_{12} = C_{13} = C_{23} = \text{diagonal}[0, 0, 1]$, with $C_{12}^2 + C_{13}^2 + C_{23}^2 = 3$, and (iii) $C_{123}^2 = 1 + 3\tau$. We note that the cusp in $S_{\max}^{(GGHZ)}$ that occurs at $\tau = 1/3$ discussed above occurs at the condition $s_1^2 + s_2^2 + s_3^2 = C_{123}^2$. For the state $|MS_3\rangle$ this latter condition would yield the unphysical result $\tau = -1$. The lesson to be learned from this non-exhaustive examination of 3-qubit pure states is that besides classifying tripartite entanglement solely in terms of the tangle, there is discriminating information to be gleaned from the distribution of the correlations amongst 1-, 2-, and 3-parties.

4. SUMMARY AND CONCLUSIONS

In this paper we have examined the structure of supra-correlations that are stronger than quantum and hence not realizable by a physical (positive) quantum state $\rho \geq 0$. The supra-correlations are intriguing because they arise from valid probability distributions, first put forth by Popescu and Rohrlich (PR), that satisfy the no-signaling principle of special relativity as well as all the usual normalization condition on the joint and marginal distributions. Thus, the fact that nature is not able to realize these supra-correlations points to hidden structure underlying how quantum correlations can be distributed amongst spacelike separated parties. This paper has examined the structure and distribution of PR correlations in 2- and 3-qubit systems by explicitly constructing “states” (not necessarily positive quantum states) that

exhibit supra-correlations for a fixed, but arbitrary number, of measurements available to each party. We have shown that the PR correlations involve only solely n -party correlations amongst the n observers. We have extended this study to include n -party correlations that capture the essential features of the PR correlations and do not rely on predetermined measurements between the n participants. By constructing constraints based on the positivity and purity of an arbitrary n -qubit state we have shown the “unreasonableness” of the PR correlations in that they encode more correlations than are physically allowed by nature. In future work we will couple this approach of studying how correlations are distributed amongst the n parties to the study of quantum entanglement. The study of entanglement²⁴ is an important, but difficult field, only well understood for the case of two qubits (both pure and mixed), and to a lesser degree, for pure 3-qubit systems. A fruitful area to investigate next are pure 3-qubit systems, where a generalized (though non-unique) Schmidt decomposition holds²⁵. We purport that an examination of the distribution of correlations, bounded by physically imposed constraints on e.g. positivity and purity, coupled with the description of entanglement in terms of the tangle, as initiated in this work, can shed further light on the classification of pure tripartite systems.

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